Chapter

2

Formulation of Optimization Problems in Chemical and Biochemical Engineering

2.1 Introduction

The major application of optimization in the chemical engineering field is minimizing energy consumption in process plant. Other applications include the optimum design of fluid flow systems, optimization of the separation process, and optimization of product concentration and reaction time in reacting systems. Estimation of the overall cost for any plant design is also a vital part. Optimization of process variables is the tool for the same. In biochemical engineering, optimization is required for finding the optimum operating conditions of a bioreactor, and parameter estimation in biochemical pathways. The process of optimization requires proper formulation of the objective function and necessary constraint functions. The objective function can be formulated in different ways based on the number of variables involve in the process. If the process mechanisms are known to us and the number of variables are less, then objective functions are formulated based on basic principles of science and technology (e.g., law of conservation, thermodynamic laws). Moreover, if the process mechanisms are complicated and not known to us, number of variables are large; statistical optimization methods like Response Surface Methodology (RSM) and Artificial Neural Network (ANN) are applicable for those processes.

2.2 Formulation of Optimization Problem

One of the important steps during the application of optimization technique to a practical problem is the formulation of objective functions. We have to develop the model equations based on the physical appearance of the system. When we are formulating the mathematical statement of the objective, we have to keep in mind that the complexity increases with the nonlinearity of the function. During optimization, more complex functions or more nonlinear functions are harder to solve. There are many modern optimization software (see chapter 12) that have been developed to solve highly nonlinear functions. Most of the optimization problems comprise one objective function. Even though some problems that involve multiple objective functions cannot be transformed into a single function with similar units (e.g., maximizing profit while simultaneously minimizing risk).

2.3 Fluid Flow System

Liquid storage and transportation trough pipeline is very common in chemical process industry. In this section, we will discuss about the design of optimization storage tank and optimum pump configuration.

2.3.1 Optimization of liquid storage tank

A cylindrical tank (Fig. 2.1) has a volume (V) that can be expressed by $V = (\pi/4)D^2L$, and we are interested to calculate the diameter (D) and height (H) that minimize the cost of the tank.

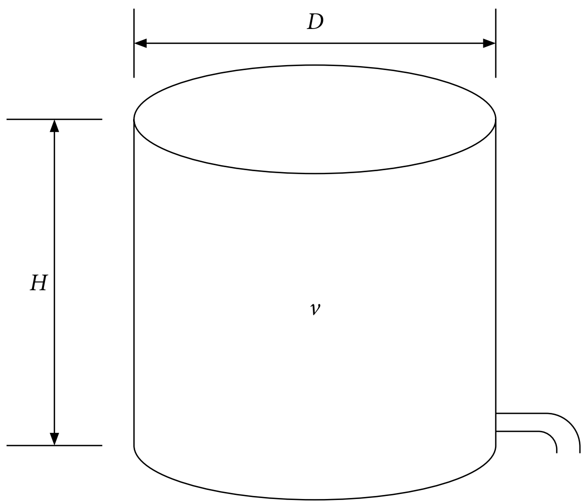

Fig. 2.1 Liquid storage tank

Cost of the tank is given by the by f; we will get the optimum design by solving the nonlinear problem:

$$\min_{H,D} f \equiv c_s \pi DH + c_t (\pi/2) D^2 \tag{2.1}$$

$$\text{subject to } V = (\pi/4) D^2 H, \tag{2.2}$$

$$D \geq 0,\; H \geq 0 \tag{2.3}$$

The cost of the tank depends on the amount of material needed which is proportional to its surface area and the cost per unit area of the tank's side is c_s, whereas for tank's top and bottom the cost per unit area is c_t.

We are able to simplify the problem by ignoring the bound constraints and eliminating the variable H from the above Eq. (2.1), giving us an unconstrained problem:

$$\min f \equiv 4c_s V/D + c_t(\pi/2)D^2 \tag{2.4}$$

Now, applying necessary condition for minimization; the objective function is differentiated with respect to D and setting the derivative to zero yields

$$\frac{df}{dD} = -4c_s V/D^2 + c_t \pi D = 0\,, \tag{2.5}$$

yielding $D = \left(\frac{4c_s V}{\pi c_t}\right)^{1/3}$, $H = \left(\frac{4V}{\pi}\right)^{1/3}\left(\frac{c_t}{c_s}\right)^{2/3}$ and the aspect ratio $H/D = c_t/c_s$.

We notice that the solution of this problem is obtained easily by using simple differential calculus. However, the generalization of this problem can make it more completed during analytical solution.

Note

The inequality constraints ($D \geq 0$, $H \geq 0$) are neglected as D and H both are positive, they remained satisfied with the solution. They are regarded as inactive constraints. If the situation were different from this case, we would need to apply more complicated optimality conditions.

We can easily eliminate one variable from the equality constraint that related H and D (Eq. (2.2)). This is often impossible for nonlinear equations and implicit elimination is required.

When we are considering these issues, particularly as they apply to very large and complicated problem, requires the numerical algorithms as discussed in chapter 3.

2.3.2 Optimization of pump configurations

There are many industries where energy consumption for fluid pumping is very high. For instance, in the pulp and paper industry, pumps consume approximately 10–20 per cent of the total electrical energy requirement. Minimization of the energy costs, as well as the total cost for the fluid pumping systems, is a major concern for these industries. In this section, we will develop the objective function for optimization of the fluid flow system. A typical problem of fluid pumping has been discussed by *T*. Westerlund *et al*. (Westerlund *et al.* 1994).

For a particular set of centrifugal pumps with given pressure rise (in terms of total head) and data for power requirement as a function of the capacity of these pumps, we have to choose the best pump or configuration of pumps coupled in parallel and/or series. This configuration should fulfill our requirements; the total required fluid flow and total pressure rise for the configuration. We are considering a very simple configuration with the total pump arranged to a L level pump configuration with $N_{p,i}$ parallel pumping lines of $N_{s,i}$ pumps in series in each line. Centrifugal pumps of the equal size and that have the same rotation speed (it may vary) are used on the same level (i). At each level, the rise in pressure head is equal to the total required pressure rise, whereas the total flow is the summation of flows through all these L levels. At each level, two real variables and two integer variables are considered for optimization. The real variables are the speed of rotation (ω_i) and the fraction (x_i) of the total flow ($\dot{V}_{\text{tot}}$). The integer variables are the number of parallel pumping lines ($N_{p,i}$) and the number of pumps in series ($N_{s,i}$). The Fig. 2.2 demonstrates an L level pump configuration.

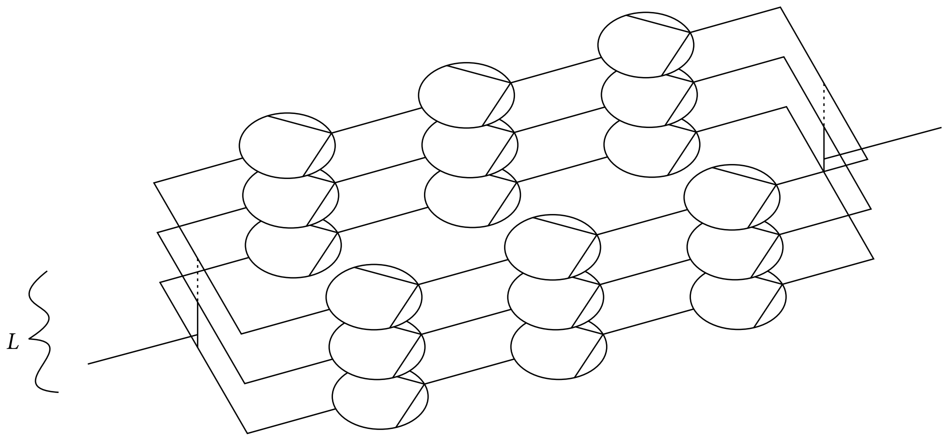

Fig. 2.2 Configuration of an L level pump network

We can represent the total cost of this pump arrangement by the following equation,

$$J = \sum_{i=1}^{L} \left(C_i + C_i' P_i \right) N_{p,i} N_{s,i} \tag{2.6}$$

where L signifies the number of levels, C_i is the yearly installment of the capital costs for a single pump, C_i' and P_i the energy and the power cost for every single pump on each level, respectively.

The power required for one pump (P_i) is usually a function of the rotational speed (ω_i) of the centrifugal pump, the flow ($\dot{V}_{\text{tot}}$) through the pump, and the density of the fluid to be pumped (ρ). Therefore, we can write

$$P_i = f_{1,i}\left(\dot{V}_i, \omega_i, \rho\right) \tag{2.7}$$

At any level i, the flow through a single pump is represented by the following equation

$$\dot{V}_i = \frac{x_i}{N_{p,i}} \dot{V}_{\text{tot}} \tag{2.8}$$

The pressure rise Δp_i is also a function of the flow ($\dot{V}_i$) through the pump and the rotational speed ω_i, as well as the fluid density (ρ); which can be written as

$$\Delta p_i = f_{2,i}\left(\dot{V}_i, \omega_i, \rho\right) \tag{2.9}$$

The rise in pressure over a single pump on each level can be demonstrated by the following equation,

$$\Delta p_i = \frac{1}{N_{s,i}} \Delta p_{\text{tot}} \tag{2.10}$$

Therefore, for a specified flow, number of pumps in series and the total rise in pressure, the rotational speed ω_i can be solved implicitly from Eqs (2.9)–(2.10). The functions, f_1 and f_2, are generally not known explicitly. However, the manufacturers are used to provide the data for power requirement and total head (pressure rise), at a constant rotational speed and a specific fluid (usually water) as a function of the capacity for a particular pump.

The data for pressure rise, given by the pump manufacturers, at a given constant rotation speed (ω_m), and for a fluid with the density (ρ_m), can be stated by the relation,

$$\Delta p_m = g_1\left(\dot{V}_m, \omega_m, \rho_m\right) \tag{2.11}$$

and the corresponding data for power requirement is given by the relation,

$$P_m = g_2\left(\dot{V}_m, \omega_m, \rho_m\right) \tag{2.12}$$

Now, by means of the proportionality relation as given in literature [Coulson and Richardsson (1985)] we get,

$$\dot{V}_i = \left(\frac{\omega_i}{\omega_m}\right) \dot{V}_m \tag{2.13}$$

$$\Delta p_i = \left(\frac{\omega_i}{\omega_m}\right)^2 \left(\frac{\rho}{\rho_m}\right) \Delta p_m \tag{2.14}$$

and

$$P_i = \left(\frac{\omega_i}{\omega_m}\right)^3 \left(\frac{\rho}{\rho_m}\right) P_m \tag{2.15}$$

Thus, the relations, $f_{1,i}$ and $f_{2,i}$, can be obtained by combining Eqs (2.13)–(2.15) with the relations, $g_{1,i}$ and $g_{21,i}$. The functions $g_{1,i}$ and $g_{21,i}$ refer to the "manufacturers" total head curve and the power curve for a particular type of pump used at level "i".

The result of the optimal configurations for pump network can be represented as MINLP problem. The statement of the optimization problem can be given as

$$\min_{N_{p,i},N_{s,i},x_i,\omega_i,i=1......L} \left\{ \sum_{i=1}^{L} \left(C_i + C_i' P_i \right) N_{p,i} N_{s,i} \right\} \tag{2.16}$$

subject to

$$\Delta p_i = f_{2,i}\left(\dot{V}_i, \omega_i\right) \tag{2.17}$$

$$\sum_{i=1}^{L} x_i = 1 \tag{2.18}$$

$$\omega_i - \omega_{i,\max} \le 0 \tag{2.19}$$

where

$$P_i = f_{1,i}\left(\dot{V}_i, \omega_i\right) \tag{2.20}$$

$$\dot{V}_i = \frac{x_i}{N_{p,i}} \dot{V}_{\text{tot}} \tag{2.21}$$

$$\Delta p_i = \frac{1}{N_{s,i}} \Delta p_{\text{tot}} \tag{2.22}$$

ω_i and x_i are non-negative real variables and the variables, $N_{p,i}$ and $N_{s,i}$, are non-negative integers.

2.4 Systems with Chemical Reaction

Optimization of product concentration is a crucial job for process engineers. Maximum amount of product will produce with minimum loss of raw materials and energy. In this section, we will discuss two different types of optimization problems in two different reacting systems.

2.4.1 Optimization of product concentration during chain reaction

For determining the optimum product concentration of any series reaction, we need to develop the mathematical equation.

A series reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ has been carried out in a PFR; where $B \rightarrow C$ is undesired reaction with unwanted product C. If we allow small time for the reaction, production of B will be very less and if we allow large time then conversion of $B \rightarrow C$ will be high. Figure 2.3 gives a clear idea about the process. It shows that at time t^* the concentration of desired product (B) will be maximum.

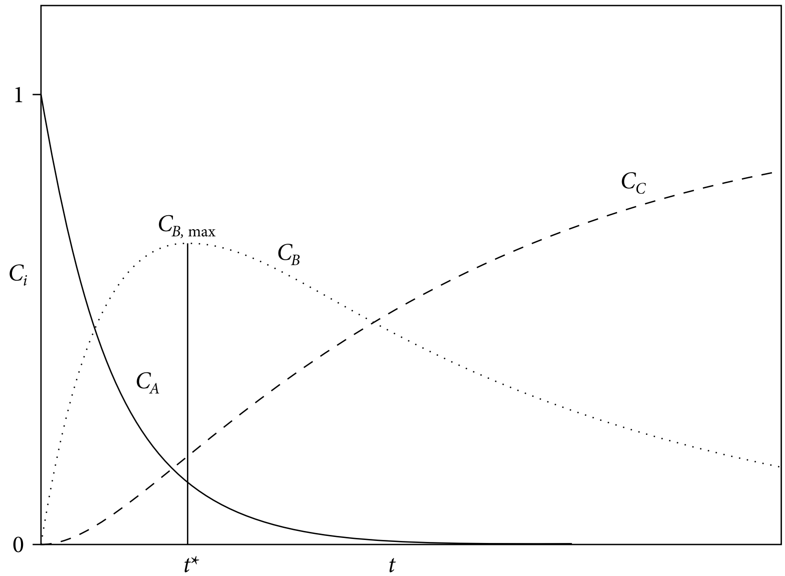

Fig. 2.3 Concentration vs. time plot for a series reaction in PFR

Now we have to develop the mathematical model equation (objective function) to find the optimum time t^*.

The rate of concentration change for A by the reaction $A \rightarrow B$ is

$$\frac{dC_A}{dt} = -r_A = -k_1 C_A \tag{2.23}$$

solving the equation we have

$$C_A(t) = C_{A_0} e^{-k_1 t} \tag{2.24}$$

the rate of concentration change for B by the reaction is

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \tag{2.25}$$

$$\frac{dC_B}{dt} = k_1 C_{A_0} e^{-k_1 t} - k_2 C_B \tag{2.26}$$

$$\frac{dC_B}{dt} + k_2 C_B = k_1 C_{A_0} e^{-k_1 t}, \tag{2.27}$$

this Eq. (2.27) is linear in C_B. Solution of this 1st order ordinary differential equation is

$$C_B(t) = C_{A_0} \frac{k_1}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) \tag{2.28}$$

This Eq. (2.28) represents the concentration of component B with time. This is a single-variable (time t) optimization problem without any constraint.

The necessary condition for finding the relative maximum is

$$\left.\frac{dC_B}{dt}\right|_{t=t^*} = 0 \tag{2.29}$$

$$\frac{dC_B}{dt} = 0 = \frac{k_1 C_{A_0}}{k_2 - k_1}\left(-k_1 e^{-k_1 t} + k_2 e^{-k_2 t}\right) \tag{2.30}$$

which gives

$$t^* = \frac{\ln\left(k_2/k_1\right)}{k_2 - k_1} \tag{2.31}$$

and

$$C_B^* = C_{A_0}\left(\frac{k_1}{k_2}\right)^{k_2/(k_2-k_1)} \tag{2.32}$$

and the sufficient condition is

$$\left.\frac{d^2 C_B}{dt^2}\right|_{t=t^*} < 0 \tag{2.33}$$

applying both necessary and sufficient condition we find the maximum concentration of component B and the optimum time t^*. This problem is considered as an isothermal PFR, if temperature changes with time objective function will change accordingly.

2.4.2 Optimization of gluconic acid production

Optimizing the production rate and product concentration in biochemical reaction is very important. In this section, we will develop a multi-objective optimization problem. This model simulates the production of gluconic acid by the fermentation of glucose in a batch stirred tank reactor using the microorganism *Pseudomona ovalis*. The mechanism of the overall biochemical reaction can be represented as follows [Johansen, T. A., and Foss, B. A. (1995)].

$$\text{Cells + Glucose + Oxygen} \rightarrow \text{More cells,} \tag{2.34a}$$

$$\text{Glucose + Oxygen} \rightarrow \text{Gluconolactone,} \tag{2.34b}$$

$$\text{Gluconolactone +Water} \rightarrow \text{Gluconic acid} \tag{2.34c}$$

The concentration of cells (X), gluconic acid (p), gluconolactone (l), glucose substrate (S), and dissolved oxygen (C) can be described by the following state-space model [Ghose, T. K., and Gosh, P. (1976)].

$$\frac{dX}{dt} = \mu_m \frac{SC}{k_s C + k_o C + SC} X \tag{2.35}$$

$$\frac{dp}{dt} = k_p l \tag{2.36}$$

$$\frac{dl}{dt} = v_l \frac{S}{k_l + S} X - 0.91 k_p l \tag{2.37}$$

$$\frac{dS}{dt} = -\frac{1}{Y_s} \mu_m \frac{SC}{k_s C + k_o C + SC} X - 1.011 v_l \frac{S}{k_l + S} X \tag{2.38}$$

$$\frac{dC}{dt} = K_L a \left(C^* - C\right) - \frac{1}{Y_o} \mu_m \frac{SC}{k_s C + k_o C + SC} X - 0.091 v_l \frac{S}{k_l + S} X \tag{2.39}$$

We can identify various objective criteria for optimizing the production of gluconic acid. Halsall-Whitney and Thibault [Hayley Halsall–Whitney and Jules Thibault (2006)] have described the multi-objective optimization scheme for this reacting system. They have concentrated on maximizing the overall rate of production (p_f / t_B) and p_f, the final concentration of gluconic acid, at the same time minimizing the concentration of final substrate (S_f) after the completion of the fermentation process. The simulations study may vary in terms of the inputs employed for defining the decision space. The choice of input variables included the duration of the fermentation process or batch time $t_B \in \left[5, 0.5h\right]$, the initial concentration of substrate $S_0 \in \left[20,0 \text{ g/L}\right]$, the concentration of initial biomass $X_0 \in \left[0.05,1.0 \text{ UOD/mL}\right]$, and the oxygen mass transfer coefficient $K_{La} \in$[50, 300 h^{-1})]. Figure 2.4 demonstrates the multi-input, multi-output optimization strategy used for optimizing the gluconic acid production.

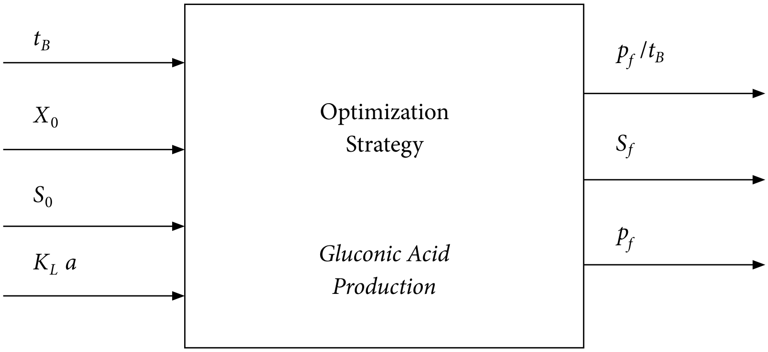

Fig. 2.4 Objectives used during optimization of gluconic acid production

2.5 Optimization of Heat Transport System

Optimization in heat transport system is required to achieve some purposes such as

i. minimize the heat loss
ii. optimum design of heat transfer equipments (e.g., heat exchanger, evaporator, condenser)
iii. optimization of Heat Exchanger Network (HEN)

2.5.1 Calculation of optimum insulation thickness

Addition of more insulation to a flat wall always decreases the heat transfer rate. The thicker the insulation, the lower the heat transfer rate. Since the area of heat transfer (A) is constant, therefore, addition of insulation always increases the thermal resistance of the wall without changing the convection resistance. However, in case of cylindrical or spherical shape, thermal resistance increases with increasing insulation thickness and convection heat transfer increases as surface area increases. Figure 2.5 shows variation of heat flux with insulation thickness. It shows that heat flux is maximum when the radius is r_{cr}. For current-carrying wires and cables, heat flux should be maximum to dissipate the heat produced. For finding the maximum heat flux and corresponding insulation thickness, we have to develop an objective function based on conduction and convection heat transfer theory.

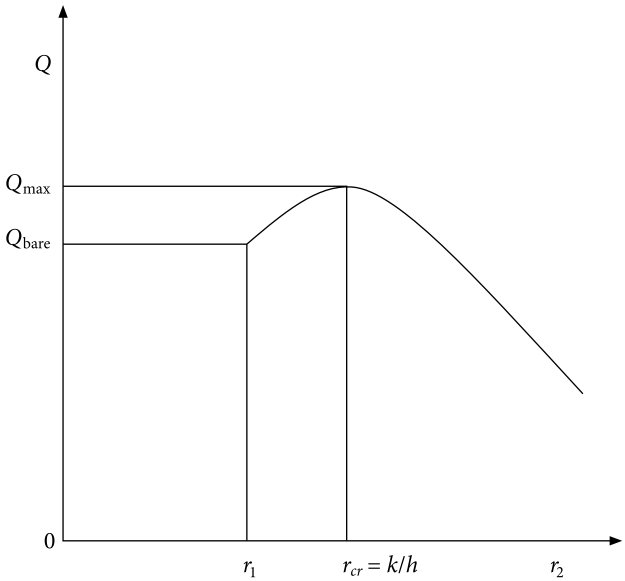

Fig. 2.5 Changes of heat flux with insulation thickness

heat transfer by conduction

$$q = \frac{2\pi Lk\left(T_i - T_o\right)}{\ln \frac{r_i}{r_o}} \tag{2.40}$$

and heat transfer by convection

$$q = 2\pi r_o Lh\left(T_o - T_\infty\right) \tag{2.41}$$

therefore, heat flux with the combined effect of conduction and convection is

$$q = \frac{T_i - T_\infty}{\frac{1}{2\pi Lk}\ln\frac{r_o}{r_i} + \frac{1}{2\pi r_o Lh}} \tag{2.42}$$

the overall resistance for heat transfer is

$$R = \frac{1}{2\pi Lk}\ln\frac{r_o}{r_i} + \frac{1}{2\pi r_o Lh} \tag{2.43}$$

To get maximum heat flux we have to minimize the overall resistance for heat transfer. This is a single-variable minimization problem where R will be minimized with respect to variable r_0. The necessary condition for solving this problem is

$$\frac{dR}{dr_o}=0 \tag{2.44}$$

$$\frac{dR}{dr_o}=\frac{d}{dr_o}\left[\frac{1}{2\pi Lk}\ln\frac{r_o}{r_i}+\frac{1}{2\pi r_o Lh}\right]=0 \tag{2.45}$$

$$\frac{1}{kr_o}-\frac{1}{hr_o^2}=0 \tag{2.46}$$

$$r_o^*=r_{cr}=\frac{k}{h} \tag{2.47}$$

The sufficient condition for this problem is

$$\frac{d^2R}{dr_o^2}=\frac{d}{dr_o}\left[\frac{1}{kr_o}-\frac{1}{hr_o^2}\right]=-\frac{1}{kr_o^2}+\frac{2}{hr_o^3}=\frac{1}{r_o^2}\left(\frac{2}{hr_o}-\frac{1}{k}\right) \tag{2.48}$$

$$\left(\frac{d^2R}{dr_o^2}\right)_{r_o=r_{cr}}=\frac{h^2}{k^2}\left(\frac{2}{k}-\frac{1}{k}\right)=\frac{h^2}{k^3}>0 \tag{2.49}$$

since, $d^2R/dr_o^2>0$, R is minimum and heat flux will be maximum

substituting the value of $r_{cr}=\dfrac{k}{h}$ in Eq. (2.43) we get the minimum value of R

$$R_{\min}=\frac{1}{2\pi Lk}\ln\frac{k}{hr_i}+\frac{1}{2\pi Lk}=\frac{1}{2\pi Lk}\left[\ln\frac{k}{hr_i}+1\right] \tag{2.50}$$

and from Eq. (2.42) we have

$$q_{\max}=\frac{2\pi Lk\left(T_i-T_\infty\right)}{\left[\ln\dfrac{k}{hr_i}+1\right]} \tag{2.51}$$

Equation 2.51 gives the maximum heat flux corresponds to critical insulation thickness.

2.5.2 Optimization of simple heat exchanger network

In this section, we are considering the optimization of a simple heat exchanger network presented in Fig. 2.6 that consists of three heat exchangers with two process streams. The process streams are defined as hot and cold streams with their inlet and outlet temperature. The hot stream that has fixed flow rate F and the heat capacity C_p requires to be cooled from T_{in} to T_{out} ($T_{in} > T_{out}$), whereas the cold stream with a fixed flow rate f and heat capacity c_p requires to be heated from t_{in} to t_{out} ($t_{out} > t_{in}$). This HE network is consists of three heat exchangers. Temperature of the steam is T_s and has a heat duty Q_b has been used by the heater, whereas the cooler with a heat duty Q_c uses cooling water at temperature T_w. However, a third heat exchanger is used to save a considerable amount of energy by transferring heat from the hot stream to the cold stream. This third heat exchanger has a heat duty Q_m with the exit temperatures of hot and cold streams, T_m and t_m, respectively.

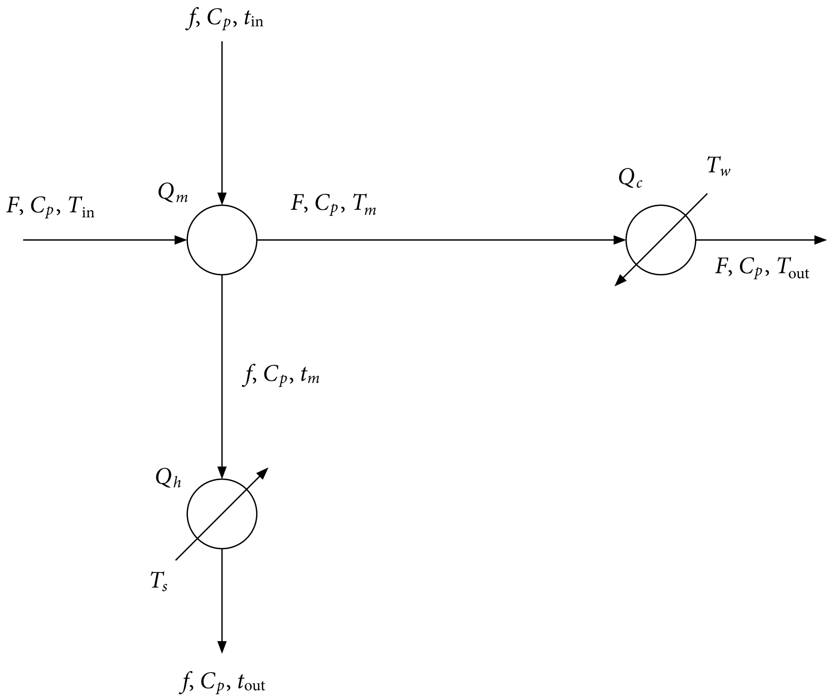

Fig. 2.6 Heat exchanger network with three heat exchangers

The model equations for this heat exchanger arrangement are described as follows:

- The energy balance equations for this HE network is represented by

$$Q_c = FC_p\left(T_{in} - T_{out}\right) \tag{2.52}$$

$$Q_b = fc_p\left(t_{out} - t_{in}\right) \tag{2.53}$$

$$Q_m = fc_p\left(t_m - t_{\text{in}}\right) = FC_p\left(T_{\text{in}} - T_m\right) \tag{2.54}$$

where the subscript c, h, and m indicate the cooler, heater and the heat exchanger.

- The capital cost of each heat exchanger depends on its area of heat exchange A_i, $i \in \{c,h,m\}$. Now we are considering a simple countercurrent, shell and tube heat exchanger that has an overall heat transfer coefficient, U_i, $i \in \{c,h,m\}$. The resultant equations for calculating the area are as follows:

$$Q_i = U_i A_i \Delta T_{lm}^i, \;\; i \in \{c,h,m\}. \tag{2.55}$$

- The log-mean temperature difference (LMTD) ΔT_{lm}^i can be written as

$$\Delta T_{lm}^i = \frac{\Delta T_a^i - \Delta T_b^i}{\ln\left(\Delta T_a^i / \Delta T_b^i\right)}, \;\; i \in \{c,h,m\}, \tag{2.56}$$

and

$$\Delta T_a^c = T_m - T_w, \;\; \Delta T_b^c = T_{\text{out}} - T_w \tag{2.57}$$

$$\Delta T_a^h = T_h - t_m, \;\; \Delta T_b^h = T_s - t_{\text{out}} \tag{2.58}$$

$$\Delta T_a^m = T_{\text{in}} - t_m, \;\; \Delta T_b^m = T_m - t_{\text{in}} \tag{2.59}$$

In this optimization problem, our intention is to minimize the total cost (the capital cost of the heat exchangers as well as the energy cost) of this HE network. This gives us the following Nonlinear Programming (NLP):

$$\min \sum_{i \in \{c,h,m\}} \left(\hat{c}_i Q_i + \bar{c}_i A_i^{\beta}\right) \tag{2.60}$$

Subject to

$$Q_c = FC_p\left(T_{\text{in}} - T_{\text{out}}\right) \tag{2.61}$$

$$Q_h = fc_p\left(t_{\text{out}} - t_{\text{in}}\right) \tag{2.62}$$

$$Q_m = fc_p\left(t_m - t_{\text{in}}\right) = FC_p\left(T_{\text{in}} - T_m\right) \tag{2.63}$$

$$Q_i = U_i A_i \Delta T_{lm}^i, \ i \in \{c,h,m\}. \tag{2.64}$$

$$\Delta T_{lm}^i = \frac{\Delta T_a^i - \Delta T_b^i}{\ln\left(\Delta T_a^i / \Delta T_b^i\right)}, \ i \in \{c,h,m\}, \tag{2.65}$$

$$Q_i \geq 0, \ \Delta T_a^i \geq \varepsilon, \ \Delta T_b^i \geq \varepsilon, \ i \in \{c,h,m\} \tag{2.66}$$

Where the cost coefficients $\hat{c}_i$ and $\overline{c}_i$ represent the energy and amortized capital prices, the exponent $\beta \in [0,1]$ represents the economy of scale of the equipment, and a small constant $\varepsilon > 0$ is chosen such that the log-mean temperature difference does not become undefined. There is one degree of freedom for this example. For example, when we specify the heat duty Q_m, the temperatures of hot and cold stream and all other remaining parameters can be estimated.

Optimization method of a heat exchanger network model has been discussed in chapter 10 (see section 10.1). The total cost of the network is optimized using superstructure optimization.

2.5.3 Maximum temperature for two rotating cylinders

Two cylinders are rotating as shown in Fig. 2.7. There is a lubricant between these cylinders. Find the maximum temperature that can be achieved in the lubricant between these two cylinders. The outer cylinder that has a radius of 8 cm rotates at an angular velocity of 9000 revolution per minute, while the inner cylinder is fixed. Clearance between the cylinders (both at 30°C) is very small, 0.025 cm. The density, viscosity, and thermal conductivity of the lubricant are 1200kg/m^3, 0.1kg/m.sec, and 0.13J/sec.m.°C respectively [Griskey, 2002].

For this system, as clearance is very small compared to their diameter, this rotating cylinders can be considered as an arrangement of two parallel plates where the upper plate (outer cylinder) moving with a velocity (the angular velocity times the radius $V_z = \Omega R$) of 12m/sec. The lower plate (inner cylinder) is fixed as shown in figure.

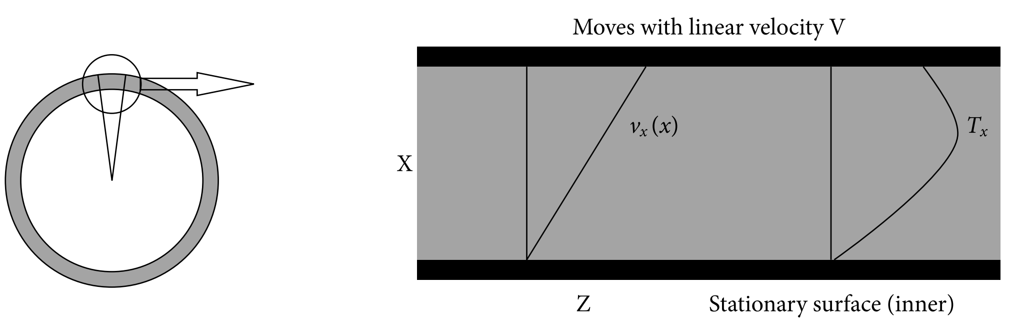

Fig. 2.7 Rotating cylinder (with temperature and velocity profile)

For the system given in Fig. 2.7, we can consider the energy balance equation and reduce it to a solvable form as described below.

The temperature profile for a Cartesian coordinate is as follows:

$$\rho \hat{C}_p \left(\cancel{\frac{\partial T}{\partial t}} + v_x \cancel{\frac{\partial T}{\partial x}} + v_y \cancel{\frac{\partial T}{\partial y}} + v_z \cancel{\frac{\partial T}{\partial z}} \right) = k \left[\frac{\partial^2 T}{\partial x^2} + \cancel{\frac{\partial^2 T}{\partial y^2}} + \cancel{\frac{\partial^2 T}{\partial z^2}} \right]$$
$$+2\mu \left\{ \left(\cancel{\frac{\partial v_x}{\partial x}} \right)^2 + \left(\cancel{\frac{\partial v_y}{\partial y}} \right)^2 + \left(\cancel{\frac{\partial v_z}{\partial z}} \right)^2 \right\} \tag{2.67}$$
$$+\mu \left\{ \left(\cancel{\frac{\partial v_x}{\partial y}} + \cancel{\frac{\partial v_y}{\partial x}} \right)^2 + \left(\cancel{\frac{\partial v_x}{\partial z}} + \frac{\partial v_z}{\partial x} \right)^2 + \left(\cancel{\frac{\partial v_y}{\partial z}} + \cancel{\frac{\partial v_z}{\partial y}} \right)^2 \right\}$$

eliminating the terms that are not required, we have

$$-k \frac{\partial^2 T}{\partial x^2} = \mu \left(\frac{\partial V_z}{\partial x} \right)^2 \tag{2.68}$$

The velocity profile can be obtained from the z component of Equation of Motion. From this equation (considering gravitational and pressure effects both zero), we get

$$\frac{\partial^2 V_z}{\partial x^2} = 0 \tag{2.69}$$

Integrating Eq. (2.69) with the boundary conditions

$$V_z = V \text{ (i.e., } \Omega R\text{)},\ x = B \tag{2.70}$$

$$V_z = 0,\ x = 0 \tag{2.71}$$

we get the relation

$$\frac{V_z}{V} = \frac{x}{B} \tag{2.72}$$

Substituting V_z from Eq. (2.72) to Eq. (2.68) we get

$$-k \frac{\partial^2 T}{\partial x^2} = \mu \frac{V^2}{B^2} \tag{2.73}$$

Now, solving Eq. (2.73) with boundary conditions

$$T = T_0,\ x = 0 \tag{2.74}$$

$$T = T_1,\ x = B \tag{2.75}$$

we obtain

$$T = T_0 + \left(T_1 - T_0\right)\frac{x}{B} + \frac{\mu V^2}{2k}\frac{x}{B}\left(1 - \frac{x}{B}\right) \tag{2.76}$$

or $$\frac{T - T_0}{T_1 - T_0} = \frac{x}{B} + \frac{\mu V^2}{2k\left(T_1 - T_0\right)}\frac{x}{B}\left(1 - \frac{x}{B}\right) \tag{2.77}$$

in the above equation, the dimensionless group is known as the Brinkman number (Br).

$$Br = \frac{\mu V^2}{k\left(T_1 - T_0\right)} = \frac{\text{Heat generated by viscous dissipation}}{\text{Conduction heat transfer}} \tag{2.78}$$

this group signifies the impact of viscous dissipation effects.

for this present case, $T_1 = T_0$ and

$$T - T_0 = \frac{\mu V^2}{2k}\frac{x}{B}\left(1 - \frac{x}{B}\right) \tag{2.79}$$

Equation (2.79) is the objective function for finding the maximum temperature. The maximum temperature will arise when $x = 0.5B$ that is, giving the largest value of $\frac{x}{B}\left(1 - \frac{x}{B}\right)$.

$$T = 30 + \frac{0.1 \times 12^2}{2 \times 0.13}\frac{1}{2}\left(1 - \frac{1}{2}\right) \tag{2.80}$$

we get the maximum temperature $T = 43.85$ °C.

2.6 Calculation of Optimum Cost of an Alloy using LP Problem

Two alloys A and B made of copper, zinc, lead, and tin are mixed to prepare C, a new alloy. The required composition of alloy C and the composition of alloys A, and B have shown in the following table (Table 2.1):

Table 2.1 Composition and cost of copper alloys

	Composition by weight			
Alloy	**Copper**	**Zinc**	**Lead**	**Tin**
A	78	12	6	4
B	62	20	16	2
C	≥ 72	≥ 15	≤ 10	≥ 3

If cost of alloy *B* is two times of alloy *A*, formulate the optimization problem for determining the amounts of *A* and *B* to be mixed to produce alloy *C* at a minimum cost.

Solution

Assume the amount of *A*, and *B* required for producing *C* are w_A and w_B respectively. And the corresponding costs per kg are c_A, and c_B. The production cost of *C* is c_C per kg.

The production cost of per kg *C* alloy is

$$c_C = c_A w_A + c_B w_B \tag{2.81}$$

We have to minimize the cost of *C* alloy

Therefore, we can write

$$\min_{w_A, w_B} c_C = c_A w_A + c_B w_B \tag{2.82}$$

with equality constraint

$$w_A + w_B = 1 \tag{2.83}$$

and inequality constraints

$$0.78 w_A + 0.62 w_B \geq 0.72 \tag{2.84}$$

$$0.12 w_A + 0.20 w_B \geq 0.15 \tag{2.85}$$

$$0.06 w_A + 0.16 w_B \geq 0.10 \tag{2.86}$$

$$0.04 w_A + 0.02 w_B \geq 0.03 \tag{2.87}$$

$$w_A, w_B, w_C \geq 0 \tag{2.88}$$

This problem can be solver using Linear Programming method.

2.7 Optimization of Biological Wastewater Treatment Plant

A rectangular tank has been made for biological treatment of wastewater (batch process). The dimensions of the tank are given in Fig. 2.8 (length x_1 meters, width x_2 meters, and height x_3 meters). The sides and bottom of the tank cost, respectively, Rs.1200/-, and Rs.2500/- per m^2 area. The operating cost for the tank is Rs.500/- for each batch of water treatment. A maintenance cost of Rs.100/- for every 10 batch is required. Assuming that the tank will have no salvage value, find the minimum cost for treatment of 1000 m^3 of wastewater. Assume the salvage value of the tank is zero after 1000 m^3 of wastewater treatment.

Solution

The total cost of water treatment =

cost of the tank + operating cost of wastewater treatment + maintenance cost

= (cost of sides + cost of bottom) + number of batch × (cost for each batch) + 100 × (number of batch)/10

$$f(X) = 1200(2x_1x_3 + 2x_2x_3) + 2500x_1x_2 + 500\left(\frac{1000}{x_1x_2x_3}\right) + 100\left(\frac{1000}{10x_1x_2x_3}\right) \tag{2.89}$$

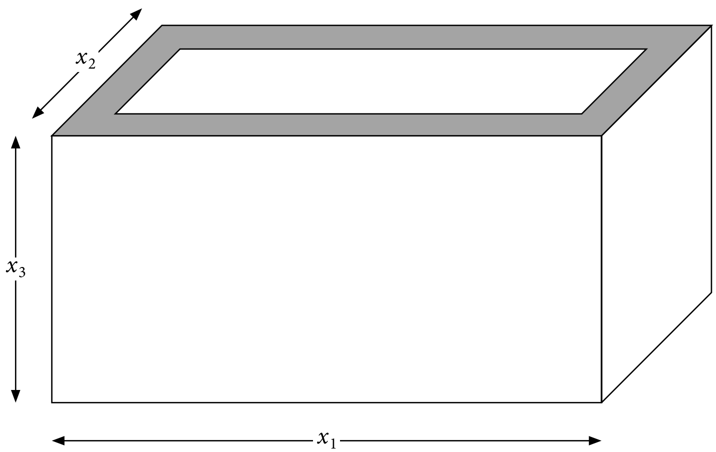

Fig. 2.8 Biological wastewater treatment plant

The above problem is an unconstrained multivariable problem that can be solve by **Geometric Programming.**

The statement of the problem is as follows:

$$\min f(X) = 1200(2x_1x_3 + 2x_2x_3) + 2500x_1x_2 + 500\left(\frac{1000}{x_1x_2x_3}\right) + 100\left(\frac{1000}{10x_1x_2x_3}\right) \tag{2.90}$$

The detail algorithm for solving this problem has been discussed in chapter 5 and chapter 9.

2.8 Calculation of Minimum Error in Least Squares Method

In many applications in chemical and biochemical engineering, we need to find the best fit curve from our experimental results. The curve of best fit is that for which e's (error values) are as small as possible i.e., E, the sum of the squares of the errors is a minimum. This is known as the principle of least squares.

Suppose it is required to fit the curve

$$y = a + bx + cx^2 \tag{2.91}$$

to a given set of observations (x_1, y_1), (x_2, y_2), …, (x_5, y_5). For any x_i, the observed value is y_i and the expected value is $\eta_i = a + bx_i + cx_i^2$ so that the error $e_i = y_i - \eta_i$ (see Fig. 2.9).

Therefore, sum of the squares of these errors is

$$E = e_1^2 + e_2^2 + \ldots + e_5^2 \tag{2.92}$$

$$E = \left[y_1 - \left(a + bx_1 + cx_1^2\right)\right]^2 + \left[y_2 - \left(a + bx_2 + cx_2^2\right)\right]^2 + \ldots + \left[y_5 - \left(a + bx_5 + cx_5^2\right)\right]^2 \tag{2.93}$$

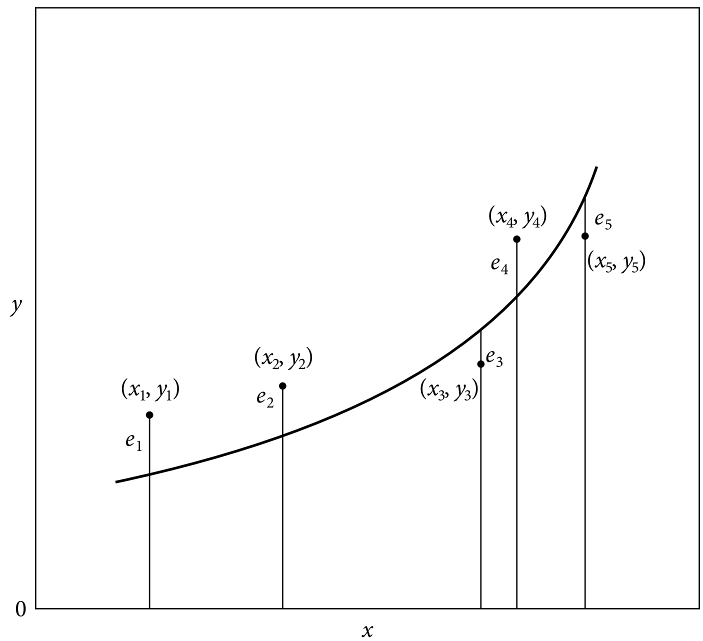

Fig. 2.9 Least square method

Equation (2.93) is the multi-variable (a, b, c) objective function from which E can be minimized.

For E to be minimum, we have

$$\frac{\partial E}{\partial a}=0=-2\left[y_1-\left(a+bx_1+cx_1^2\right)\right]-2\left[y_2-\left(a+bx_2+cx_2^2\right)\right]-\ldots -2\left[y_5-\left(a+bx_5+cx_5^2\right)\right] \tag{2.94}$$

$$\frac{\partial E}{\partial b}=0=-2x_1\left[y_1-\left(a+bx_1+cx_1^2\right)\right]-2x_2\left[y_2-\left(a+bx_2+cx_2^2\right)\right]-\ldots -2x_5\left[y_5-\left(a+bx_5+cx_5^2\right)\right] \tag{2.95}$$

$$\frac{\partial E}{\partial c}=0=-2x_1^2\left[y_1-\left(a+bx_1+cx_1^2\right)\right]-2x_2^2\left[y_2-\left(a+bx_2+cx_2^2\right)\right]-\ldots -2x_5^2\left[y_5-\left(a+bx_5+cx_5^2\right)\right] \tag{2.96}$$

Equation (2.94) simplifies to

$$y_1+y_2+\ldots+y_5=5a+b\left(x_1+x_2+\ldots+x_5\right)+c\left(x_1^2+x_2^2+\ldots+x_5^2\right) \tag{2.97}$$

$$\sum_{i=1}^{5}y_i=5a+b\sum_{i=1}^{5}x_i+c\sum_{i=1}^{5}x_i^2 \tag{2.98}$$

Equation (2.95) becomes

$$x_1y_1+x_2y_2+\ldots+x_5y_5=a\left(x_1+x_2+\ldots+x_5\right)+b\left(x_1^2+x_2^2+\ldots+x_5^2\right) +c\left(x_1^3+x_2^3+\ldots+x_5^3\right) \tag{2.99}$$

$$\sum_{i=1}^{5}x_iy_i=a\sum_{i=1}^{5}x_i+b\sum_{i=1}^{5}x_i^2+c\sum_{i=1}^{5}x_i^3 \tag{2.100}$$

Similarly, (2.96) simplifies to

$$\sum_{i=1}^{5}x_i^2y_i=a\sum_{i=1}^{5}x_i^2+b\sum_{i=1}^{5}x_i^3+c\sum_{i=1}^{5}x_i^4 \tag{2.101}$$

The Eqs (2.98), (2.100), and (2.101) are known as Normal equations and can be solved as simultaneous equations in a, b, c. The values of these constants when substituted in Eq. (2.91) give the desired curve of best fit.

For n number of data point similar equations can be written as

$$\sum_{i=1}^{n} y_i = na + b\sum_{i=1}^{n} x_i + c\sum_{i=1}^{n} x_i^2 \tag{2.102}$$

$$\sum_{i=1}^{n} x_i y_i = a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i^3 \tag{2.103}$$

$$\sum_{i=1}^{n} x_i^2 y_i = a\sum_{i=1}^{n} x_i^2 + b\sum_{i=1}^{n} x_i^3 + c\sum_{i=1}^{n} x_i^4 \tag{2.104}$$

a, b, c are found from these equations.

2.9 Determination of Chemical Equilibrium

The following example is used to explain the application of nonlinear programming in chemical engineering. A mixture of various chemical compounds has been considered for this study. The problem on chemical equilibrium is proposed by Bracken and McCormick [Bracken and McCormick (1968)]. This problem is to define the mixture composition of different chemicals when the mixture is at the state of chemical equilibrium. According to the second law of thermodynamics, the free energy of a mixture of chemicals reaches its minimum value at a constant temperature and pressure when the mixture is in chemical equilibrium condition. Therefore, by minimizing the free energy of the mixture, we can determine the chemical composition of any mixture satisfying the state of chemical equilibrium. For describing this system, we will consider the following notations as given below

m : number of chemical elements in the mixture

n : number of compounds in the mixture

x_j: number of moles for compound j, $j = 1, \ldots, n$

s : total number of moles in mixture, $s = \sum_{i=1}^{n} x_j$

a_{ij} : number of atoms of element i in a molecule of compound j

b_i : atomic weight of element i in the mixture $i = 1, \ldots, n$

The constraint equations for the mixture are given below. All compounds should have a nonnegative number of moles.

$$x_j \geq 0 \text{ , } j = 1, \ldots, n \tag{2.105}$$

There is a material balance equation for each element. These equations are represented by linear equality constraint.

$$\sum_{j=1}^{n} a_{ij} x_j = b_i \text{ , } i = 1, \ldots, m \tag{2.106}$$

Here, the total free energy of the mixture is the objective function

$$f(x) = \sum_{j=1}^{n} x_j \left[c_j + \ln\left(\frac{x_j}{s} \right) \right] \tag{2.107}$$

where

$$c_j = \left(\frac{F^0}{RT} \right)_j + \ln(P) \tag{2.108}$$

and $\left(F^0/RT\right)_j$ is the model standard free energy function for the jth compound. P represents the total pressure in atmospheres. Our aim is to find out the parameters x_j that minimize the objective function $f(x)$ subject to the constraints non-negativity of mole number (as given by Eq. (2.105)) and linear balance (as given by Eq. (2.106)). Therefore, the optimization problem can be written as

$$\text{Min } f(x) = \sum_{j=1}^{n} x_j \left[c_j + \ln\left(\frac{x_j}{s} \right) \right] \tag{2.107}$$

$$\text{subject to: } c_j = \left(\frac{F^0}{RT} \right)_j + \ln(P) \tag{2.108}$$

$$\sum_{j=1}^{n} a_{ij} x_j = b_i, \ i = 1, \ldots, m \tag{2.106}$$

$$x_j \geq 0, \ j = 1, \ldots, n \tag{2.105}$$

Further study

Readers can find some advanced topic for further studies.

i. Optimization of energy consumption in refinery (Gueddar and Dua, 2012)

ii. Global optimization of pump configurations using Binary Separable Programming (Pettersson and Westerlund, 1997)

iii. Optimization of a large scale industrial reactor by genetic algorithms (Rezende *et al.* 2008)

iv. Economic Process Optimization Strategies (Buskies, 1997)

Summary

- This chapter gives us an idea about the formulation of the optimization problem. Various chemical engineering systems have been presented in this chapter. Optimization problems for fluid flow system, heat transport systems, and reactor systems are formulated to maximize the efficiency of the system. Optimization of composition during alloy preparation and blending is very crucial job for chemical engineers. We have discussed the optimization problem on alloy preparation. This chapter also includes optimization of biological wastewater treatment plant, parameter estimation using least square method, determination of chemical equilibrium. The solutions of the aforementioned are discussed in the subsequent chapters.

Exercise

Problem 2.1

We are interested to produce P in the reaction $A \rightarrow P$ using a continuous reactor at v = 240 liters/hr with $C_{A_0} = 3$ moles/liter. However, it is noticed that there is a second reaction $P \rightarrow R$ that can also occur. This undesired reaction produced undesired product R. It is found that both reactions are irreversible and first order with k_1 = 0.45 min^{-1} and k_2 = 0.1 min^{-1}. Derive the objective function for finding maximum yield of P.

Problem 2.2

For installation and operation of a pipeline for an incompressible fluid, the total cost (in dollars per year) can be represented as follows:

$$C = C_1 D^{1.5} L + C_2 m \Delta p / \rho$$

where

C_1 = the installed cost of the pipe per foot of length computed on an annual basis ($C_1 D^{1.5}$ is expressed in dollars per year per foot length, C_2 is based on \$0.05/kWh, 365 days/year and 60 percent pump efficiency).

D = diameter (to be optimized)

L = pipeline length = 100 miles

m = mass flow rate = 200,000 lb/h

$\Delta p = \left(2\rho v^2 L / D g_c\right) f$ = pressure drop, psi

ρ = density = 60 lb/ft3

v = velocity = $(4m)/\left(\rho \pi D^2\right)$

f = friction factor = $\left(0.046\mu^{0.2}\right)/\left(D^{0.2} v^{0.2} \rho^{0.2}\right)$

μ = viscosity = 1 cP

a. Find general expressions for D^{opt}, v^{opt}, and C^{opt}

b. For $C_1 = 0.3$ (D expressed in inches for installed cost), calculate D^{opt} and v^{opt} for the following pairs of values of μ and ρ; $\mu = 0.2, 10$ cP, $\rho = 50, 80$ lb/ft^3

Problem 2.3

A fertilizer producing company purchases nitrates, phosphates, potash, and an inert chalk base and produces four different fertilizers A, B,C, and D. The cost of these nitrates, phosphates, potash, and an inert chalk base are \$1600, \$550, \$1100, and \$110 per ton, respectively. The cost of production, selling price, and composition of the four fertilizers are given in the following table.

Table 2.2 Cost of production, selling price, and composition of fertilizers

Fertilizer	Production cost (\$/ton)	Selling price (\$/ton)	Percentage composition by weight			
			Nitrates	Phosphates	Potash	Inert chalk base
A	98	340	4.5	10	5.5	80
B	155	560	6	15	9	70
C	260	720	14	6	15	65
D	195	440	10	18	10	62

The supply of nitrates, phosphates, and potash is limited, no more than 1100 tons of nitrate, 2200 tons of phosphates, and 1600 tons of potash will be available for a week. The company is required to supply to its customers a minimum of 5200 tons of fertilizer A and 4100 tons of fertilizer D per week; however, it is otherwise free to produce the fertilizers in any quantities it satisfies. Formulate the problem (objective function and constrained functions) to find the quantity of each fertilizer to be produced by the company that maximize its profit.

Problem 2.4

Heavy fuel oil, initially semisolid at 15^{0}C is to be heated and pumped through a 15 cm diameter (inside) pipe at the rate of 20000 kg/h. The pipe line is 1500 long and efficiently lagged. The cost of power for pumping is Rs.1.0 per kwh used with 50 per cent efficiency, while the cost of steam heat is Rs.40.0 per million kilocalorie. On the basis of the following data, calculate the economic (optimum) pumping temperature.

Data: Specific heat of oil = 0.5 kcal/kg ^{0}C ; Density of oil = 950 kg/m^3

$H_{fs} = \dfrac{2 f v^2 L}{gcD}$ where $f = 4 \times Re^{-0.2}$, Re = Reynolds Number

Oil viscosity (kg/m.sec) $\mu = \dfrac{1.0}{dT}$

Where dT is the rise in oil temperature over 15°C

Problem 2.5

The topological optimization is discussed in chapter 1. Here, we will consider a topological optimization problem for a chemical process plant. The layout of the chemical process plant has been shown in Fig.

2.10. This plant consists of a water tank (*T*), a pump (*P*), a fan (*F*), and a compressor (*C*). The positions of the different units are also indicated in this figure in terms of their (*x*, *y*) coordinates. It has been decided to add a new heat exchanger (*H*) within this plant. Addition of new unit may cause congestion within the plant. It is decided to place *H* within a rectangular area given by $\{-15 \le x \le 15, -10 \le y \le 10\}$ to avoid congestion. Formulate the optimization problem to find the position of *H* to minimize the sum of its distances *x* and *y* from the existing units, *T*, *P*, *F*, and *C*.

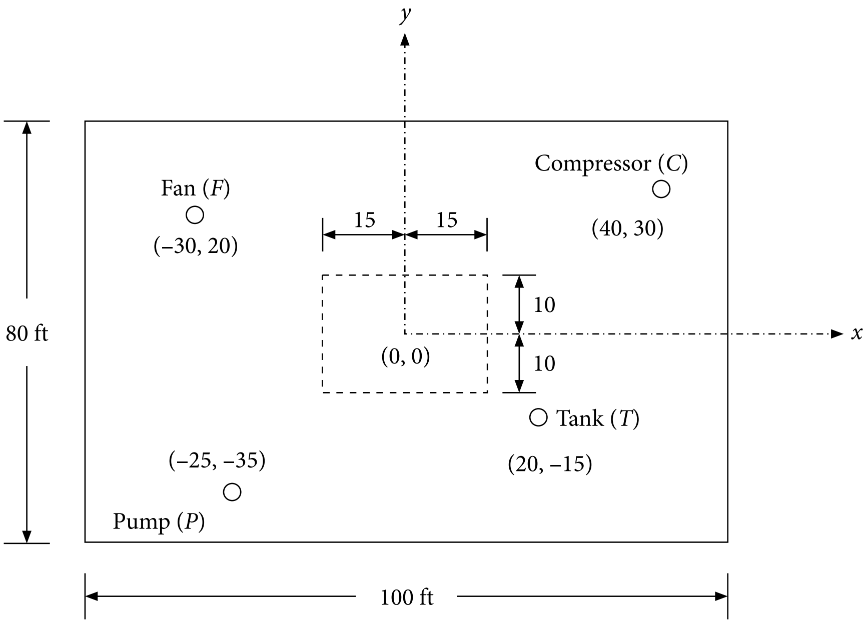

Fig. 2.10 Layout of a chemical processing plant (coordinates in ft)

Problem 2.6

Two grade of coal (*A*, *B*) are mixed to get a coal (*C*) for blast furnace. The composition of coals and cost of coals are given in the table below

Table 2.3 Composition and cost of coal

Coal	Composition (%) and cost (per ton) of coal			
	Carbon	Sulphur	Ash	Cost per ton
A	92	1	7	Rs. 2000/-
B	81	2	17	Rs. 1500/-
C	≥ 88	≤ 1.5	≤ 10	

Develop the optimization problem to determine the amounts of *A* and *B* to be mixed to produce *C* at a minimum cost.

Problem 2.7

An oil refinery has three process plants, and four grades of motor oil have been produced from these plants. The refinery is liable to meet the demand of customers. The refinery incurs a penalty for failing to meet the demand for any particular grade of motor oil. The capacities of the various plants, the costs of production, the demands of motor oil of the different grades, and the penalties have shown in the following table:

Table 2.4 The details of various plants

Process plant	Plant capacity (kgal/day)	Cost of production ($/day)			
		1	2	3	4
1	100	800	900	1000	1200
2	150	850	950	1150	1400
3	200	900	1000	1250	1600
Demand (kgal/day)		45	140	100	70
Penalty (for shortage of each kilogallon)		$9	$12	$15	$21

Formulate the optimization problem as an LPP for minimizing the overall cost.

Problem 2.8

An adiabatic two-stage compressor is used to compress a gas, which is cooled to the inlet gas temperature between the stages, the theoretical work can be expressed by the following equation:

$$W = \frac{kp_1V_1}{k-1}\left[\left(\frac{p_2}{p_1}\right)^{(k-1)/k} - 2 + \left(\frac{p_3}{p_2}\right)^{(k-1)/k}\right]$$

Where, $k = C_p/C_v$; p_1 = pressure inlet; p_2 = intermediate stage pressure; p_3 = outlet pressure; V_1 = inlet volume

We are interested to optimize the intermediate pressure p_2 such that the work is a minimum.

Problem 2.9

A refinery produce three major products: gasoline, jet fuel and lubricants by distilling crude petroleum from two sources, Venezuela and Saudi Arabia. These two crudes have different chemical composition and therefore, provide different product mixes. From one barrel of Saudi crude, 0.25 barrel of gasoline, 0.45 barrel of jet fuel, and 0.2 barrel of lubricants are produced. Whereas, one barrel of Venezuelan crude produces 0.4 barrel of gasoline, 0.2 barrel of jet fuel, and 0.3 barrel of lubricants. The refinery losses 10 per cent of each barrel during the crude refining.

The crudes also differ in cost and availability: Up to 9,000 barrels per day of Saudi crude are available at the cost $20 per barrel; Up to 6,000 barrels per day of Saudi crude are also available at the lower cost $15 per barrel. The refinery has contracts with independent distributors to supply 2,000 barrels of gasoline per day, 1,500 barrels of jet fuel per day, and 500 barrels of lubricants per day. Formulate an optimization model in standard form to fulfill the requirements in the most efficient manner.

Problem 2.10

A chemical company has acquired a site for their new plant. They required to enclose that field with a fence. They have 700 meter of fencing material with a building on one side of the field where fencing is not needed. Determine the maximum area of the field that can be enclosed by the fence.

References

Bracken, J. and McCormick, G. P. 1968. *Selected Applications of Nonlinear Programming*, New York : John Wiley and Sons.

Buskies, U. 'Chemical Engineering Technology' *Economic Process Optimization Strategies,* 20(1997) 63–70.

Coulson, J. M. and Richardson, J. F. 1985. *Chemical Engineering*, vol. 1, Oxford: Pergamon Press.

Edgar, T. F., Himmelblau D. M., Lasdon L. S. *Optimization of Chemical Processes* (2e), New York: McGraw–Hil.

Ghose, T. K. and Gosh, P. (1976). 'Kinetic Analysis of Gluconic Acid Production by Pseudomonas Ovalis', *Journal of Applied Chemical Biotechnology*, 26, 768–77.

Grewal, B. S. *Higher Engineering Mathematics* (37e), Delhi-110006: Khanna Publishers, India.

Griskey, R. G. 2002. *Transport Phenomena and Unit Operations*: A Combined Approach, New York: John Wiley and Sons.

Gueddar, T., Dua V. *Novel model reduction techniques for refinery-wide energy optimization*, Applied Energy, 89(2012): 117–26.

Halsall–Whitney, H., Thibault, J. *Multi-Objective Optimization for Chemical Processes and Controller Design: Approximating and Classifying the Pareto Domain*, Computers and Chemical Engineering, 30(2006): 1155–68.

Johansen, T. A. and Foss, B. A. (1995). *Semi-Empirical Modeling of Non-linear Dynamic Systems through Identification of Operating Regimes and Locals Models*. In K. Hunt, G. Irwin, and K. Warwick (Eds.), Neural Network Engineering in Control Systems, Springer–Verlag, pp. 105–26.

Levenspiel, O. *Chemical Reaction Engineering* (3*e*), New Jersey: John Wiley and Sons, Inc.

Peters, M. S., Timmerhaus, K., West, R. E. *Plant Design and Economics for Chemical Engineers* (5*e*), New York: McGraw–Hil.

Pettersson, F. and Westerlund, T. 1997. *Global Optimization of Pump Configurations Using Binary Separable Programming*, Computers Chemical Engineering, vol. 21, No. 5, pp. 521–29.

Rao, S. S. *Engineering Optimization Theory and Practice*, Fourth Edition, New Jersey: John Wiley and Sons, Inc.

Rezende, M. C. A. F., Costa C. B. B., Costa A. C., Maciel M. R. W., Filho R. M. *Optimization of a Large Scale Industrial Reactor by Genetic Algorithms*, Chemical Engineering Science, 63(2008): 330–41.

Roy, G. K. 2000. *Solved Examples in Chemical Engineering* (7*e*), Delhi: Khanna Publishers

Schmidt, L. D. 2005. *The Engineering of Chemical Reactions* (2*e*), New York: Oxford University Press.

Westerlund, T., Pettersson, F., Grossmann, I. E. 1994. *Optimization of Pump Configurations as a MINLP Problem*, Computers Them. Engng., vol. 18, No. 9, pp. 845–58.